Marie-Liesse Doublet

List of Publications by Year
in descending order

114 papers	9,440 citations	71102 41 h-index	37204 96 g-index
122 all docs	122 docs citations	122 times ranked	8708 citing authors

#	Article	IF	Citations
1	Advancement of the Homogeneous Background Method for the Computational Simulation of Electrochemical Interfaces. Journal of Chemical Theory and Computation, 2022, 18, 1883-1893.	5.3	9
2	Chemical Design of IrS₂ Polymorphs to Understand the Charge/Discharge Asymmetry in Anionic Redox Systems. Chemistry of Materials, 2022, 34, 325-336.	6.7	1
3	Access to Ru(IV)â€“Ru(V) and Ru(V)â€“Ru(VI) Redox in Layered Li₇RuO₆ via Intercalation Reactions. Chemistry of Materials, 2022, 34, 3724-3735.	6.7	3
4	The Irâ€“OOOOâ€“Ir transition state and the mechanism of the oxygen evolution reaction on IrO₂(110). Energy and Environmental Science, 2022, 15, 2519-2528.	30.8	40
5	Elucidation of Active Oxygen Sites upon Delithiation of Li₃IrO₄. ACS Energy Letters, 2021, 6, 140-147.	17.4	12
6	Unlocking anionic redox activity in O3-type sodium 3d layered oxides via Li substitution. Nature Materials, 2021, 20, 353-361.	27.5	155
7	Investigation of alkali and alkaline earth solvation structures in tetraglyme solvent. Physical Chemistry Chemical Physics, 2021, 23, 26120-26129.	2.8	7
8	Activation of anionic redox in d0 transition metal chalcogenides by anion doping. Nature Communications, 2021, 12, 5485.	12.8	26
9	Stacking Versatility in Alkali-Mixed Honeycomb Layered NaKNi₂TeO₆. Inorganic Chemistry, 2021, 60, 14310-14317.	4.0	9
10	Correlating ligand-to-metal charge transfer with voltage hysteresis in a Li-rich rock-salt compound exhibiting anionic redox. Nature Chemistry, 2021, 13, 1070-1080.	13.6	75
11	The Structural Stability of P2-Layered Na-Based Electrodes during Anionic Redox. Joule, 2020, 4, 420-434.	24.0	89
12	Unveiling Pseudocapacitive Charge Storage Behavior in FeWO₄ Electrode Material by Operando Xâ€Ray Absorption Spectroscopy. Small, 2020, 16, e2002855.	10.0	16
13	Thermodynamic origin of dendrite growth in metal anode batteries. Energy and Environmental Science, 2020, 13, 5186-5197.	30.8	101
14	Unexpected band gap increase in the Fe2VAl Heusler compound. Materials Today Physics, 2020, 13, 100203.	6.0	20
15	Electrolyte Reactivity in the Double Layer in Mg Batteries: An Interface Potential-Dependent DFT Study. Journal of the American Chemical Society, 2020, 142, 5146-5153.	13.7	71
16	New p-type Al-substituted SrSnO₃ perovskites for TCO applications?. Chemical Communications, 2020, 56, 2566-2569.	4.1	7
17	Charge Transfer Band Gap as an Indicator of Hysteresis in Li-Disordered Rock Salt Cathodes for Li-Ion Batteries. Journal of the American Chemical Society, 2019, 141, 11452-11464.	13.7	81
18	Unified picture of anionic redox in Li/Na-ion batteries. Nature Materials, 2019, 18, 496-502.	27.5	335

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19	Zn_{0.35}Co_{0.65}O â€“ A Stable and Highly Active Oxygen Evolution Catalyst Formed by Zinc Leaching and Tetrahedral Coordinated Cobalt in Wurtzite Structure. Advanced Energy Materials, 2019, 9, 1900328.	19.5	41
20	A Chemical Approach to Raise Cell Voltage and Suppress Phase Transition in O3 Sodium Layered Oxide Electrodes. Advanced Energy Materials, 2018, 8, 1702599.	19.5	127
21	Electrochemical Mg alloying properties along the Sb1-xBix solid solution. Electrochimica Acta, 2018, 259, 276-283.	5.2	30
22	Electrostatic Interactions versus Second Order Jahnâ€“Teller Distortion as the Source of Structural Diversity in Li₃MO₄ Compounds (M = Ru, Nb, Sb and Ta). Chemistry of Materials, 2018, 30, 392-402.	6.7	15
23	Atomic Structure of 2 nm Size Metallic Cobalt Prepared by Electrochemical Conversion: An in Situ Pair Distribution Function Study. Journal of Physical Chemistry C, 2018, 122, 23861-23866.	3.1	14
24	Competition between Metal Dissolution and Gas Release in Li-Rich Li₃Ru_yIr_{1â€“y}O₄ Model Compounds Showing Anionic Redox. Chemistry of Materials, 2018, 30, 7682-7690.	6.7	25
25	Reversible Sodium and Lithium Insertion in Iron Fluoride Perovskites. Advanced Functional Materials, 2018, 28, 1802057.	14.9	33
26	Chemical Activity of the Peroxide/Oxide Redox Couple: Case Study of Ba₅Ru₂O₁₁ in Aqueous and Organic Solvents. Chemistry of Materials, 2018, 30, 3882-3893.	6.7	8
27	The Electrochemical Sodiation of Sb Investigated by Operando X-ray Absorption and 121Sb MÃ¶ssbauer Spectroscopy: What Does One Really Learn?. Batteries, 2018, 4, 25.	4.5	20
28	Evidence for anionic redox activity in a tridimensional-ordered Li-rich positive electrodeÂÎ²-Li2IrO3. Nature Materials, 2017, 16, 580-586.	27.5	290
29	Requirements for reversible extra-capacity in Li-rich layered oxides for Li-ion batteries. Energy and Environmental Science, 2017, 10, 266-274.	30.8	269
30	Activation of surface oxygen sites on an iridium-based model catalyst for the oxygen evolution reaction. Nature Energy, 2017, 2, .	39.5	435
31	The electrochemical activity of the nitrosyl ligand in copper nitroprusside: a new possible redox mechanism for lithium battery electrode materials?. Electrochimica Acta, 2017, 257, 364-371.	5.2	15
32	Approaching the limits of cationic and anionic electrochemical activity with the Li-rich layered rocksalt Li3IrO4. Nature Energy, 2017, 2, 954-962.	39.5	138
33	A₂VO(SO₄)₂ (A = Li, Na) as Electrodes for Li-Ion and Na-Ion Batteries. Chemistry of Materials, 2016, 28, 6637-6643.	6.7	22
34	Strong Oxygen Participation in the Redox Governing the Structural and Electrochemical Properties of Na-Rich Layered Oxide Na₂IrO₃. Chemistry of Materials, 2016, 28, 8278-8288.	6.7	132
35	A Fully Ordered Triplite, LiCuSO₄F. Chemistry of Materials, 2016, 28, 1607-1610.	6.7	9
36	The intriguing question of anionic redox in high-energy density cathodes for Li-ion batteries. Energy and Environmental Science, 2016, 9, 984-991.	30.8	453

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37	Atomistic Modeling of Electrode Materials for Li-Ion Batteries: From Bulk to Interfaces. Green Energy and Technology, 2016, , 1-36.	0.6	2
38	Visualization of O-O peroxo-like dimers in high-capacity layered oxides for Li-ion batteries. Science, 2015, 350, 1516-1521.	12.6	659
39	Influence of polymorphism on the electrochemical behavior of M Sb negative electrodes in Li/Na batteries. Journal of Power Sources, 2015, 280, 695-702.	7.8	21
40	Origin of the Voltage Hysteresis of MgH₂ Electrodes in Lithium Batteries. Journal of Physical Chemistry C, 2015, 119, 17044-17052.	3.1	37
41	Reversible Li-Intercalation through Oxygen Reactivity in Li-Rich Li-Fe-Te Oxide Materials. Journal of the Electrochemical Society, 2015, 162, A1341-A1351.	2.9	47
42	Li2Cu2O(SO4)2: a Possible Electrode for Sustainable Li-Based Batteries Showing a 4.7 V Redox Activity vs Li+/Li0. Chemistry of Materials, 2015, 27, 3077-3087.	6.7	31
43	Origin of voltage decay in high-capacity layered oxide electrodes. Nature Materials, 2015, 14, 230-238.	27.5	757
44	An intuitive and efficient method for cell voltage prediction of lithium and sodium-ion batteries. Nature Communications, 2014, 5, 5559.	12.8	39
45	New Insights on the Reversible Lithiation Mechanism of TiO₂(B) by Operando X-ray Absorption Spectroscopy and X-ray Diffraction Assisted by First-Principles Calculations. Journal of Physical Chemistry C, 2014, 118, 27210-27218.	3.1	23
46	An Oxysulfate Fe2O(SO4)2 Electrode for Sustainable Li-Based Batteries. Journal of the American Chemical Society, 2014, 136, 12658-12666.	13.7	16
47	Conceptual Surface Electrochemistry and New Redox Descriptors. Journal of Physical Chemistry C, 2014, 118, 19023-19031.	3.1	31
48	Reversible anionic redox chemistry in high-capacity layered-oxide electrodes. Nature Materials, 2013, 12, 827-835.	27.5	1,192
49	An ab initio study of surface electrochemical disproportionation: The case of a water monolayer adsorbed on a Pd(111) surface. Catalysis Today, 2013, 202, 87-97.	4.4	55
50	High Performance Li₂Ru_{1â€“y}Mn_yO₃ (0.2 â‰¤ Tj ETQq0 0 0 rgBT /O Chemistry of Materials, 2013, 25, 1121-1131.	6.7	365
51	Palladiumâ€“Silver Mesowires for the Extended Detection of H₂. ACS Applied Materials & Interfaces, 2013, 5, 310-318.	8.0	18
52	Origin of the Voltage Hysteresis in the CoP Conversion Material for Li-Ion Batteries. Journal of Physical Chemistry C, 2013, 117, 837-849.	3.1	87
53	Li4NiTeO6 as a positive electrode for Li-ion batteries. Chemical Communications, 2013, 49, 11376.	4.1	96
54	Single-Step Synthesis of FeSO₄F_{1â€“y}OH_y (0 â‰¤ y) Tj ETQq0 0 0 rgBT /Ov	6.7	35

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55	Origin of the 3.6 V to 3.9 V voltage increase in the LiFeSO4F cathodes for Li-ion batteries. Energy and Environmental Science, 2012, 5, 9584.	30.8	58
56	A 3.90 V iron-based fluorosulphate material for lithium-ion batteries crystallizing in the triplite structure. Nature Materials, 2011, 10, 772-779.	27.5	301
57	Interface electrochemistry in conversion materials for Li-ion batteries. Journal of Materials Chemistry, 2011, 21, 10134.	6.7	66
58	FeII/FeIII mixed-valence state induced by Li-insertion into the metal-organic-framework Mil53(Fe): A DFT+U study. Journal of Power Sources, 2011, 196, 3426-3432.	7.8	51
59	Crystal structure, band structure and electrical properties of Î²-(BEDT-TTF)2SbF6 grown on a Si(001) electrode. Synthetic Metals, 2010, 160, 556-560.	3.9	3
60	Design of Electrode Materials for Lithium-Ion Batteries: The Example of Metalâ^'Organic Frameworks. Journal of Physical Chemistry C, 2010, 114, 9518-9527.	3.1	82
61	Interplay between Magnetic and Orbital Ordering in the Strongly Correlated Cobalt Oxide: A DFTâ€‰+â€‰U Study. Journal of Physical Chemistry C, 2010, 114, 21750-21756.	3.1	32
62	P-Redox Mechanism at the Origin of the High Lithium Storage in NiP2-Based Batteries. Chemistry of Materials, 2009, 21, 298-308.	6.7	71
63	Updated references for the structural, electronic, and vibrational properties of TiO2(B) bulk using first-principles density functional theory calculations. Journal of Chemical Physics, 2009, 130, 204501.	3.0	99
64	Structural, magnetic and redox properties of a new cathode material for Li-ion batteries: the iron-based metal organic framework. Ionics, 2008, 14, 279-283.	2.4	34
65	Redox mechanism in the NiP2 electrode for Li-ion batteries: A DFT study coupled with local chemical bond analyses. Ionics, 2008, 14, 197-202.	2.4	8
66	Phase Diagrams for Systems with Low Free Energy Variation:â€‰ A Coupled Theory/Experiments Method Applied to Li-Graphite. Journal of Physical Chemistry C, 2008, 112, 3982-3988.	3.1	37
67	Direct Correlation between the ³¹P MAS NMR Response and the Electronic Structure of Some Transition Metal Phosphides. Journal of Physical Chemistry C, 2008, 112, 20481-20490.	3.1	47
68	Determination of Lithium Insertion Sites in LixTiP4(x= 2â^'11) by Electron Energy-Loss Spectroscopy. Journal of Physical Chemistry C, 2007, 111, 3996-4002.	3.1	19
69	Electrical Conductivity and Spin Crossover:â€‰ A New Achievement with a Metal Bis Dithiolene Complex. Inorganic Chemistry, 2007, 46, 8548-8559.	4.0	104
70	Mixed-Valence Li/Fe-Based Metalâ€“Organic Frameworks with Both Reversible Redox and Sorption Properties. Angewandte Chemie - International Edition, 2007, 46, 3259-3263.	13.8	583
71	FeP:â€‰ Another Attractive Anode for the Li-Ion Battery Enlisting a Reversible Two-Step Insertion/Conversion Process. Chemistry of Materials, 2006, 18, 3531-3538.	6.7	181
72	Redox mechanism in the binary transition metal phosphide Cu3P. Journal of Physics and Chemistry of Solids, 2006, 67, 1252-1257.	4.0	47

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73	(BETS)2[RuX5NO] (X = Cl, Br): An Explanation of Different Conductive Properties Through Structural and Spectroscopic Studies. Journal of Low Temperature Physics, 2006, 142, 449-452.	1.4	0
74	(BETS)2[RuX5NO] (X=Cl, Br): an explanation of different conductive properties through structural and spectroscopic studies. Journal of Low Temperature Physics, 2006, 142, 445-448.	1.4	1
75	Electrochemical Behaviors of Binary and Ternary Manganese Phosphides.. ChemInform, 2006, 37, no.	0.0	0
76	On the Reactivity of Li8-yMnyP4 Toward Lithium.. ChemInform, 2005, 36, no.	0.0	0
77	Progress in the lithium insertion mechanism in Cu3P. Ionics, 2005, 11, 36-45.	2.4	19
78	Leading interactions in theÎ²â^'SrV6O15compound. Physical Review B, 2005, 71, .	3.2	34
79	On the Reactivity of Li8-yMnyP4 toward Lithium. Chemistry of Materials, 2005, 17, 3627-3635.	6.7	33
80	Electrochemical Reactivity and Design of NiP2 Negative Electrodes for Secondary Li-Ion Batteries. Chemistry of Materials, 2005, 17, 6327-6337.	6.7	229
81	Electrochemical Behaviors of Binary and Ternary Manganese Phosphides. Chemistry of Materials, 2005, 17, 5817-5823.	6.7	57
82	Redox-Induced Structural Change in Anode Materials Based on Tetrahedral (MPn4)x- Transition Metal Pnictides.. ChemInform, 2004, 35, no.	0.0	0
83	The LixMPn4 phases (M/Pn = Ti/P, V/As): new negative electrode materials for lithium ion rechargeable batteries. Electrochimica Acta, 2004, 49, 2325-2332.	5.2	49
84	Redox-Induced Structural Change in Anode Materials Based on Tetrahedral (MPn4)x- Transition Metal Pnictides. Chemistry of Materials, 2004, 16, 1002-1013.	6.7	63
85	Lithium insertion/deinsertion mechanisms in the transition metal pnictides LixMPn4. Ionics, 2003, 9, 56-63.	2.4	9
86	The LixVPn4Ternary Phases (Pn: P, As): Rigid Networks for Lithium Intercalation/Deintercalation.. ChemInform, 2003, 34, no-no.	0.0	0
87	New salts derived from organic donor molecules with long-living excited states counter-ions. Synthetic Metals, 2003, 133-134, 377-380.	3.9	1
88	The LixVPn4 Ternary Phases (Pn = P, As):â€‰ Rigid Networks for Lithium Intercalation/Deintercalation. Chemistry of Materials, 2002, 14, 4126-4133.	6.7	61
89	Similarities between the t-J and Hubbard models in weakly correlated regimes. European Physical Journal B, 2002, 28, 49-54.	1.5	2
90	Synthesis, electrical behaviour, and crystal and electronic band structures of two different phases of the (SMeEt2)[Pd(dmit)2]2 salt. Consequences of cationic disorder on the electrical properties. Journal of Materials Chemistry, 2001, 11, 2205-2210.	6.7	8

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91	Structure and properties of BETS salts: Î º-(BETS)8(Cu2Cl6)(CuCl4), Î¸-(BETS)2(CuCl2) and (BETS)2(CuCl4). Comptes Rendus De L'Academie Des Sciences - Series IIc: Chemistry, 2001, 4, 149-160.	0.1	1
92	Anion Conformation and Physical Properties in BETS Salts with the Nitroprusside Anion and its Related Ruthenium Halide (X = Cl, Br) Mononitrosyl Complexes: Î¸-(BETS)4[Fe(CN)5NO], (BETS)2[RuBr5NO], and (BETS)2[RuCl5NO]. European Journal of Inorganic Chemistry, 2001, 2001, 2797.	2.0	25
93	Density functional theory analysis of the local chemical bonds in the periodic tantalum dichalcogenides TaX2 (X=S,â€ŠSe,â€ŠTe). Journal of Chemical Physics, 2000, 113, 5879-5890.	3.0	29
94	Correlation and dimerization effects on the physical behavior of the NR4[Ni(dmit)2]2 charge transfer salts: A density matrix renormalization group study of the quarter-filling tâ€“J model. Journal of Chemical Physics, 1999, 110, 1767-1773.	3.0	6
95	Why has 1T-TaTe2 not yet been synthetized? A DFT contribution.. Synthetic Metals, 1999, 103, 2679-2682.	3.9	3
96	Quantitative on-site repulsion U for the Ni(dmit)2 molecule: A DMRG study of the NR4[Ni(dmit)2]2 salts. Synthetic Metals, 1999, 103, 2062-2063.	3.9	0
97	A new theoretical approach for the electrical properties of TiX2 (X=S, Se, Te) phases with density functional calculations. Journal of Chemical Physics, 1998, 108, 649-658.	3.0	11
98	Metallic conductivity in a disordered charge-transfer salt derived from cis-BET-TTF. Synthetic Metals, 1997, 86, 2145-2146.	3.9	16
99	Electronic Structure of the $mathsf{alpha}$-(BEDT-TTF)$mathsf{_2}$MHg(XCN)$mathsf{_4}$ (Mâ€‰=â€‰Tl,) Tj ETQq1 1 0.7843 Organic Metal $alpha$-(BEDT-TTF)$mathsf{_2}$TlHg(Se$mathsf{_{m 1-x}}$S$mathsf{_{m) Tj ETQq1 1 0.784314 rgBT /Overlock 10	1.2	30
100	Effect of the cooling rate on the transverse magnetoresistance of (TSeT)2Cl in its charge-density wave ground state. Physica B: Condensed Matter, 1995, 211, 286-289.	2.7	2
101	H2O photodissociation dynamics based on potential energy surfaces from density functional calculations. Journal of Chemical Physics, 1995, 103, 2538-2547.	3.0	13
102	Structural and electronic properties of the molecular conductors (EDTTTF)x[Pd(dmit)2]y(x:y=2:3 and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.8	11
103	A New Family of Molecular Metals Based on Bis(ethylenethio)tetrathiafulvalene (BET-TTF) and Octahedral Counterions. Chemistry of Materials, 1995, 7, 1558-1567.	6.7	28
104	Interplay between structural, magnetic properties and calculated band structures of (EDT-TTF)2[M(dmit)2]2 where M = Ni, Pd. Synthetic Metals, 1995, 70, 1063-1064.	3.9	4
105	Magnetoresistance in pulsed fields, band structure calculations and charge-density wave instability in (TSeT)2Cl. Synthetic Metals, 1995, 70, 1279-1280.	3.9	4
106	Electronic properties of isostructural organic conductors (ET)3(HSO4)2 and [Ni(dddt)2]3(HSO4)2. Thermopower and tight-binding calculations. Synthetic Metals, 1995, 71, 1867-1868.	3.9	5
107	Concerning the first-order transition in the ?-phase (BEDT-TTF)4PtCl6 . C6H5CN. Journal De Physique, I, 1994, 4, 1479-1490.	1.2	24
108	Comparison of the electronic structures of isostructural (BEDT-TTF)3(HSO4)2 and [Ni(dddt)2] 3(HSO4)2 molecular metals. Journal De Physique, I, 1994, 4, 1439-1450.	1.2	8

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109	Structure-Property Correlations in the Platinum Oxide and Palladium Sulfide Bronzes with Columnar Chains of Square-Planar TX4 Units (T = Pt, X = O; T = Pd, X = S). Journal of the American Chemical Society, 1994, 116, 2115-2120.	13.7	17
110	The Mechanism of Acetylene Cyclotrimerization Catalyzed by the fac-IrP3+ Fragment: The Relationship between Fluxionality and Catalysis. Organometallics, 1994, 13, 2010-2023.	2.3	62
111	Synthesis, Crystal Structure, Electrical Properties and Electronic Band Structure of (NHyMe4-y)x[M(dmit)2] Complexes (M = Ni, Pd, Pt; dmit2- = 2-Thioxo-1,3-dithiole-4,5-dithiolato). Inorganic Chemistry, 1994, 33, 3401-3414.	4.0	42
112	Factors affecting the metallic versus semiconducting properties of charge transfer salts containing [M(dddt)2]2 and [M(dmit)2]2 (M = Pd, Pt) dimers. Solid State Communications, 1993, 88, 699-703.	1.9	25
113	Inhibited superconductivity induced by localization effects in (EDT-TTF)2[Pd(dmit)2]2. Synthetic Metals, 1993, 56, 2833-2838.	3.9	6
114	Comparison of the electronic structures of the BEDT-TTF4[M(CN)4] (M = Ni, Pt) and BEDT-TTF4[M(C2O4)2] (M = Pt, Cu) salts. Structural requirements for hidden Fermi surface nesting. Journal De Physique, I, 1993, 3, 2451-2461.	1.2	5